Numerical Modelling for Phase Changing Materials (PCM)

Alice Raeli, Mejdi Azaïez, Michel Bergmann, Angelo Iollo

Numerical Modelling for Phase Changing Materials (PCM)

Alice Raeli
Mejdi Azaïez, Michel Bergmann, Angelo Iollo.
Department of Mathematics, Bordeaux

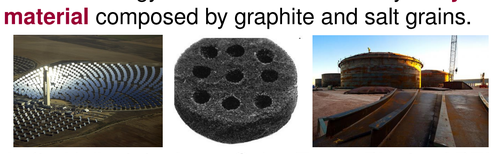
alice.raeli@math.u-bordeaux1.fr

Abstract

There are several reasons for a numerical study of partial differential equations; many of them describe physical phenomena such as electromagnetism, elasticity, etc... In this work we present an approach for the heat equation with discontinuous conductivity and its relative boundary conditions. We present a finite difference method (FDM) on hierarchical meshes based on octrees (quadtrees for 2D cases) built to solve the mathematical model that describes a Phase Changing Material (PCM). We show an analysis of this method and its building reasons; then we describe the technical tools and necessary observations for a consistent cell centered method. The mesh refinement follows the hybrid material's interface looking for the accuracy on the discontinuity presented by the physical problem.

1. Problem

ABENGOA Solar is focused on renewable and sustainable energy. In this work we study a **hybrid material** composed by graphite and salt grains.

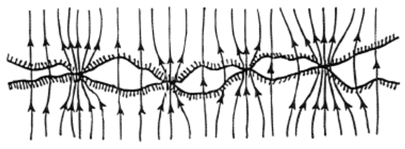


Left: Heliostats Area, Solar Tower Plant - ABENGOA Solar (Sevilla, Spain). Center: Phase Changing Material. Right: Tank containing the PCM.
The heat is conserved in the tank and it causes the salt grains to liquefy, generating the initial energy storage. Later, the solidification transfers this heat to release the stored energy.

2. Mathematical Hybrid Model

Let G be the graphite and S be the PCM.
$k = (k_S(T), k_G)$ is the thermal conductivity.

$$\begin{aligned} \partial_t H(T) - \nabla \cdot (\kappa \nabla T) &= g \\ \kappa \partial_n T &= 0 \qquad (\Gamma_N) \\ T &= T_D \qquad (\Gamma_D) \\ [\kappa \partial_n T] = 0 \qquad (\kappa \partial_n T)_G &= \frac{1}{R}[T] \quad (\gamma) \\ T(0) &= 0 \qquad (\Omega) \end{aligned}$$



The holes generated by the phase change generate a discontinuity of temperature, depending on a constant contact resistance; however the flux conservation condition ensures the continuity of the normal derivatives.

The **enthalpy function** is strictly connected to a function that describes the phase change:

$$H(T) = \begin{cases} [(\rho C)^s_S(1 - f(T)) + (\rho C)^l_S f(T))]T & \\ +\rho^l_S f(T) L_a & \text{in S} \\ (\rho C)_G T & \text{in G} \end{cases}$$

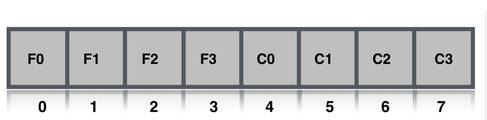
$$f(T) = \frac{1}{2}(1 + \tanh \frac{T - T_F}{\delta T})$$

3. Octrees discretization tools

A quadtree is 2:1 balanced if any two neighboring nodes differ by at most 1 in depth. We suppose here to work on a quadtree-based 2D discretization. The grids we refer to in this work are graded on faces and edges with a maximal jump of two levels on the vertices. The same reasons can be developed in the 3D cases.

Definition 3.1 *A linear octree is an octree that is represented by a linear array instead of a tree data structure. Its structure allows an efficient memory saving (this advantage is commonly used in adaptive mesh refinement and coarsening (AMR) algorithms).*

Quadtree type discretizations seem intuitive for spatial distribution topology but not easy to manage. A first necessity for the treated linear octree discretization was the identification of all possible configurations. We used a Z-order method for the grids that allows us to obtain a unique way case by case. We choose a base-5 8-digits numerical key (resp. 26-digits for 3D case) built looking at neighbours configuration of each octant following the curve orientation (example in figure).



2D key order where F stands for face and C for corner.

Using a proper functional based on the levels $[L] = L - nL$, with L the level of the concerned octant and nL the level of the neighbour, the value attribution on the key elements follows:

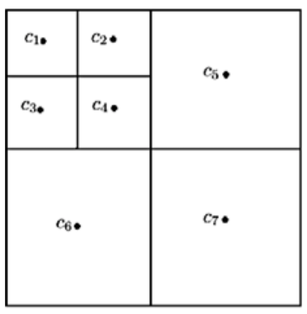
0	∄ neighbours in this side
1	$[L] = 0$
2	$[L] = -1$
3	$[L] = 1$
4	$[L] = -2$
5	$[L] = 2$

4. Elements of an octree based cell centered FDM

Definition 4.1 (Consistency) *A finite difference scheme is said to be consistent with the partial differential equation it represents, if for any sufficiently smooth solution u of this equation, the truncation error of the scheme tends uniformly towards zero with respect to x, when h tends to zero, i.e. if:*

$$\lim_{h \to 0} ||\epsilon_h||_\infty = 0$$

Moreover, if there exists a constant $C > 0$, such that $||\epsilon_h|| < C^p$, with $p > 0$, then the scheme is said to be accurate at the order p.



First example reference configuration. The concerned point is c_4.

For a cell centered finite difference method we start by an example (in figure) presented in [1] for the interested reader.
Let h be the side lenght of the cell with center c_4, with a neighbours analysis it is simple to deduce the projected distances on x and y directions from c_4 to the neighbours centers with dependence on h. Let $u(P)$ be the solution function and a_i the weights of the finite difference method of concerned points in a configuration; the a_i are obtained such that $\sum_{i=1}^{7} a_i u_i = u_{xx}(c_4) + u_{yy}(c_4)$ where the u_i terms are obtained by taylor series expansions centered on the relative point.
A first result (Min et al.) is:

Theorem 4.1 *Consider the discretization of the Poisson equation at the center of the cell c_4. If only face-adjacent cells are to be used, then there does not exist any locally consistent linear scheme on non-uniform Cartesian grids.*

This result is obtained by solving the sistem of the six relative constraints for the concistency. We can observe that the totality of concerned points with an edges implementation is seven so we can determine infinite solutions of the complete system:

$$\begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & -h & 0 & -h & \frac{3h}{2} & -\frac{h}{2} & \frac{3h}{2} \\ 0 & h & h & 0 & \frac{h}{2} & -\frac{3h}{2} & -\frac{3h}{2} \\ 0 & \frac{h^2}{2} & 0 & \frac{h^2}{2} & \frac{9h^2}{8} & \frac{h^2}{8} & \frac{9h^2}{8} \\ 0 & -h^2 & 0 & 0 & \frac{3h^2}{4} & \frac{3h^2}{4} & -\frac{9h^2}{4} \\ 0 & \frac{h^2}{2} & \frac{h^2}{2} & 0 & \frac{h^2}{8} & \frac{9h^2}{8} & \frac{9h^2}{8} \end{pmatrix} \begin{pmatrix} a_4 \\ a_1 \\ a_2 \\ a_3 \\ a_5 \\ a_6 \\ a_7 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 1 \end{pmatrix}$$

For a described mesh the number of constraints is 6 (10 on 3D case) for the consistency, and the number of neighbours in any involved configuration is from 7 to 13; consequently the system requiring the consistency admits a solution for a stencil that involves all the neighbours of a centered point. For a unique solution we need:

- a way to identify uniquely any configuration (the chosen key presented above);
- additional constraints that ensure a solution.

5. The additional constraints

The idea is to ensure the consistency and minimize the deviation from second order as best as possible. Let M be the constraint matrix, $\vec{\omega}$ the weights, $\vec{\lambda}$ the necessary additional unknowns, $\vec{f}$ the right hand side vector for consistency and $F(\vec{\omega})$ a weight function. The problem to minimize has the lagrangian form:

$$\mathcal{L} = F(\vec{\omega}) - \lambda(M\vec{\omega} - f) \qquad (1)$$

$$\Downarrow$$

$$\frac{\partial \mathcal{L}}{\partial \omega} = 0 \Rightarrow \frac{\partial F(\omega)}{\partial \omega} - M^T \vec{\lambda} = 0$$
$$\frac{\partial \mathcal{L}}{\partial \lambda} = 0 \Rightarrow M\vec{\omega} = f$$

We write minimization problem (1) in matrix form, let be:

- x the vector that includes the weights and the λ added terms, b the right hand side vector that includes the consistency parameters ($\vec{f}$) and 0 for the other additional equations.
- A the final problem matrix for searching the configuration's weights, B the matrix obtained by imposing the 6 constraints of consistency, C the submatrix of the 4 constraints with third order derivatives, I a large enough identity matrix.

$$Ax = b \Leftrightarrow \begin{cases} \frac{\partial F(\omega)}{\partial \omega} - M^T \vec{\lambda} & = 0 \\ M\vec{\omega} & = f \end{cases}$$

Two cases have to be distinguished for N the number of concerned points in a configuration:

- $N \leq 10: \quad M = B$
  $F(\omega) = 1/2((1-\alpha)C^T C - \alpha I)\omega^T \omega$

$$Ax = \begin{pmatrix} ((1-\alpha)C^T C - \alpha I) & -B^T \\ B & 0 \end{pmatrix} x = b$$

  Ensured 6 constraints for consistency imposition and minimization of second order constraints and weights norm.

- $N > 10: \quad M = \binom{B}{C} \quad F(\omega) = 1/2(\omega^T \omega)$

$$Ax = \begin{pmatrix} I & -\binom{B}{C}^T \\ \binom{B}{C} & 0 \end{pmatrix} x = b$$

  Ensured 10 constraints for second order imposition and minimization of the weights norm.

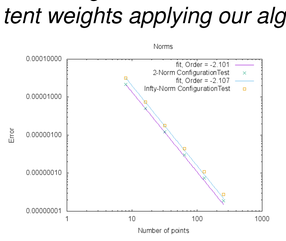
Remark 5.1 *The consistency constraints for the 3D cases is 10 and the total number of equations for the second order accuracy is 20. Consequently the two cases are $N \leq 20$ and $N > 20$.*

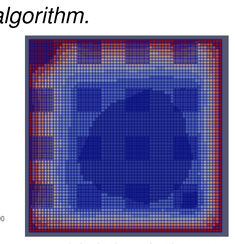
6. Algorithm steps

- to identify the configuration on each octant;
- to build the weights matrix and keep the solution;
- to build the system of PDE solver matrix with the relative weights and data octant by octant line;
- solve the system with an assigned source term function and extract the numerical solution of the problem.

7. Numerical Results: Application of the Finite Element Method

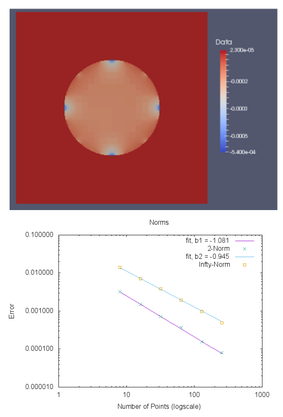
Test 7.1 (Configuration Test) *A first test is built on the configuration test where we looked for consistent weights applying our algorithm.*





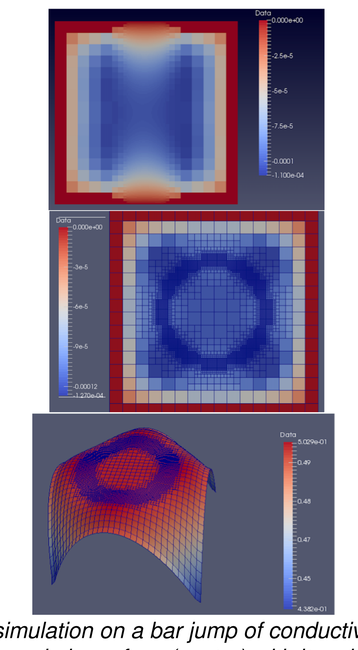
Order (left) and a result error (right) of the test configuration presented in [1] (dark blue stands for $-7e-06$).

Test 7.2 (Penalization Method) *We established consistency and convergence of the method testing random grids (we suppose that we do not know a priori the molten salt disposition in the graphite structure), then we supposed that the salt has a circle composition and we focused on surface and internal part (subject to phase change) ignoring the graphite that has constant properties. So we applied the penalization method to improving a local concentration of variables approaching the heat problem of the material on microscopic way.*



Error example (top) and method order (bottom): the order 1 was expected from theory.

Test 7.3 (Discontinuity Simulation) *We simulated the discontinuity of the conductivity k using a mollified heaviside function on more different surfaces for a jump from 1 to 1 million on a small number of cells, we established a control for the jump modifying his width and the related cells.*



Error simulation on a bar jump of conductivity (top) and on a circle surface (center) with its relative numerical solution (bottom).

Current Works and Future Plans

Currently the same examples are replicated in 3D cases to confirm the validity of the method and to complete this part. The number of variables concerned on the weights systems is different but the complete algorithm follows the same steps until the Poisson solver. In a second moment we will apply the method to real variables of the material problem (we remark that the material exists and its conductivity properties are known) studying the phase change to optimize the energy storage for the molten salt. In addition with this work we expect to be able to perform a reduction order model for a faster solver dedicated to PCM equations.

References

[1] Min et al., A supra-convergent finite difference scheme for the variable coefficient Poisson equation on non-graded grids, Journal of Computational Physics 218 (2006).